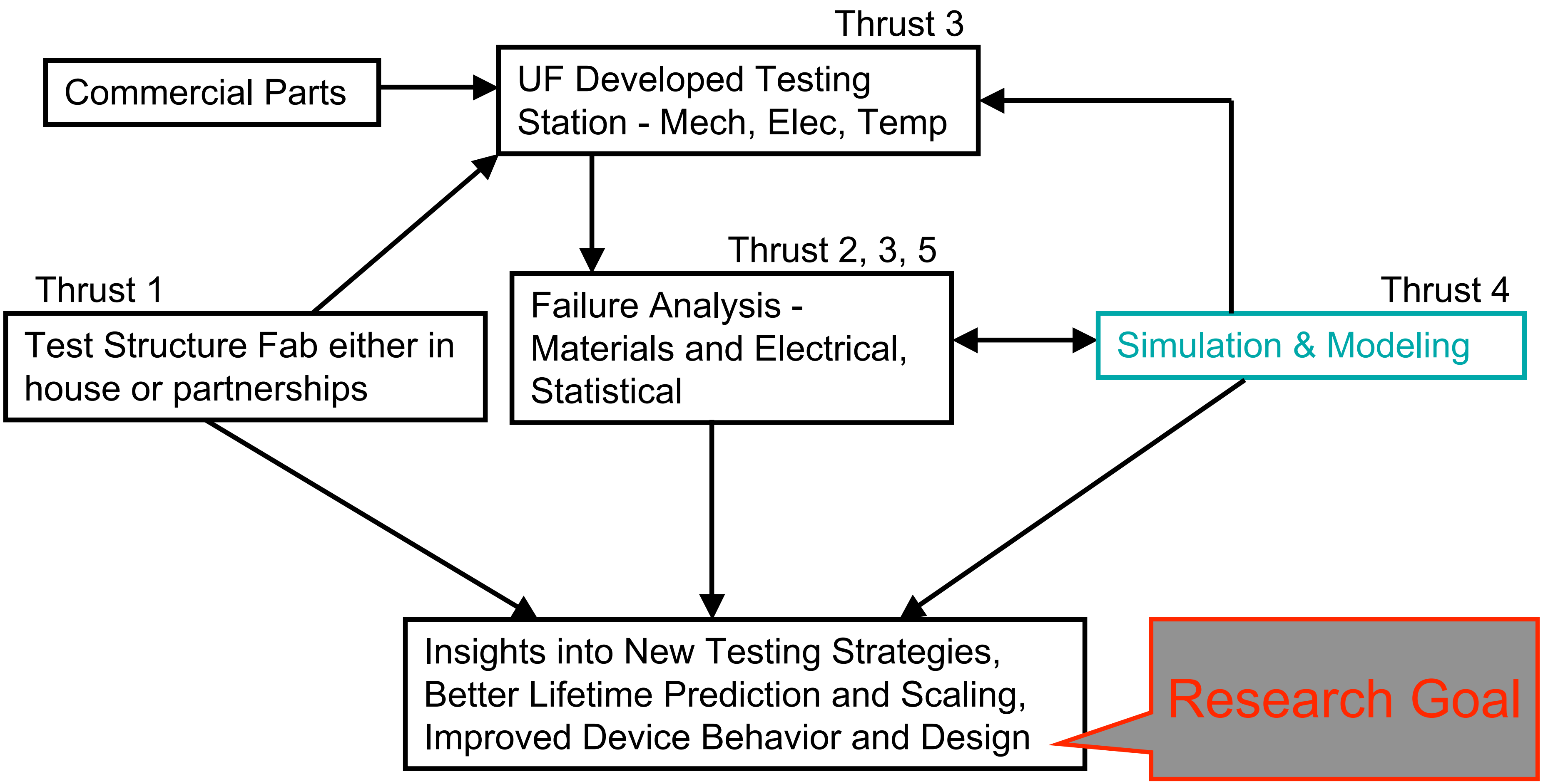
Overview of Modeling and Simulation

Drs. Law, Bosman, Nishida, Thompson

Outline

- Modeling Overview
- Strain Effects
- Noise Modeling
- Device Simulation Development
- Directions

Research Work Plan



FLOOPS / FLOODS

- Object-oriented codes
- Multi-dimensional
- P = Process / D = Device 90% code shared
- Scripting capability for PDE's - Alagator

- Commercialized - ISE / Synopsis
  - Sentaurus - Process is based on FLOOPS
- Licensed at over 300 sites world-wide
  - 2008 release
  - Manual is online (building a wiki manual)

What is Alagator?

- Scripting language for PDE's
- Parsed into an expression tree
- Assembled using FV / FE techniques
- Stored in hierarchical parameter data base

- Models are accessible, easily modified

What is Alagator?

Operator	*Description*
"ddt"	Time derivative
"grad"	Spatial derivative
"sgrad"	Scharfetter / Gummel Discretization Operator
"dot"	Returns the dot product of the gradient of two field – electric field in direction of current flow
"elastic"	Compute elastic forces - FEM balance

- Example use of operators for diffusion equation
- Fick's Second Law of Diffusion
  - ddt(Boron) - 9.0e-16 * grad(Boron) - K * (Boron - Trap)
  - $\partial C(x,t) / \partial t = D \partial^2 C(x,t) / \partial x^2$

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Simulation Capability — Band Structure

– Tight binding method.

✓ relatively simple and gives whole band structure
✓ straightforward microscopic picture of how strain affects inter-atomic interactions

– k·p method.

✓ semi-empirical parameters for greater accuracy at the Γ point
✓ physical parameters such as momentum-matrix elements and eigen-energies
✓ strain effect incorporated through **deformation potential**

We heavily use k·p method [1] since it is semi-empirical and more accurate provided accurate deformation potentials are used.

- effective mass
- mobility enhancement
- threshold voltage shift
- gate leakage change

1 [Opt Quant Electron, vol. 40, pp. 295, 2008]

k·p Method for Wurtzite Crystal

The Hamiltonian $$H = H_0 + \frac{\hbar^2 k^2}{2m_0} + H_{so} + \frac{\hbar}{m_0} k \ p + H_{strain}$$

Conduction and valence bands Hamiltonian

- Conduction band (parabolic band model)

$$H^c(k_t, k_z) = (\frac{\hbar^2}{2})(\frac{k_t^2}{m_e^t} + \frac{k_z^2}{m_e^z}) + E_c + H_{strain}$$

- Valence band

$$H_{6\times6}{}^v(k) = \begin{bmatrix} H_{3\times3}^U(k) & 0 \\ 0 & H_{3\times3}^L(k) \end{bmatrix} + H_{strain}$$

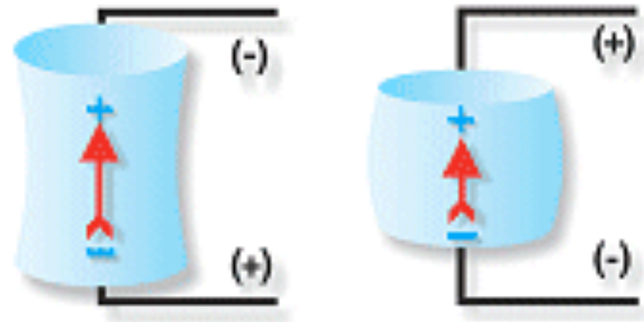
where $$H_{3\times3}^U(k) = \begin{bmatrix} F & K_t & -iH_t \\ K_t & G & \Delta - iH_t \\ iH_t & \Delta + iH_t & \lambda \end{bmatrix}$$ and $$H_{3\times3}^L(k) = conj(H_{3\times3}^U(k))$$

[Phys. Rev. B, 54, 2491 (1996)]

Deformation potential basis to construct the strain Hamiltonian

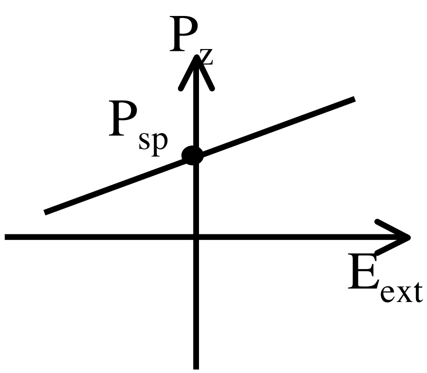
Strain Induced by Inverse Piezoelectricity

Inverse Piezoelectricity: Strain actuated by applied electric field



1) Applied electric field E_{ext}

2) $E_{ext} \rightarrow$ Polarization P_z



3) $P_z \rightarrow$ In-plane strain ϵ_{xx}

$$\begin{pmatrix} P_x \\ P_y \\ P_z \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{zx} \\ \varepsilon_{xy} \end{pmatrix}$$

$$\varepsilon_{xx} = \varepsilon_{yy} = \frac{C_{33}}{2\left(e_{31}C_{33} - e_{33}C_{13}\right)} P_z$$

GaN: $e_{31} = -0.32 \quad e_{33} = 0.63$

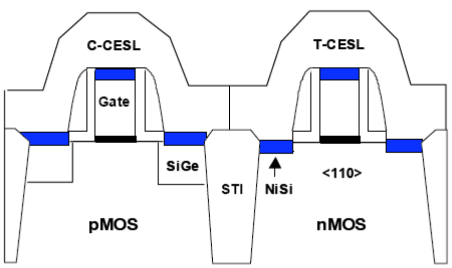
AlN: $e_{31} = -0.38 \quad e_{33} = 1.29$

Under typical HEMT operation bias (V_{DG}~20V), additional strain induced by inverse piezoelectricity is around 0.1% (500MPa).

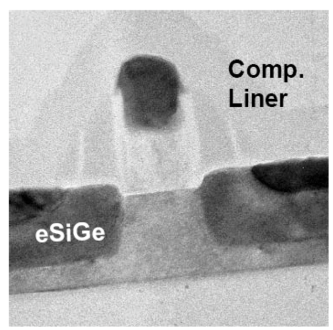
[JAP, vol. 84, pp. 4951, 1998]

Strained PMOS

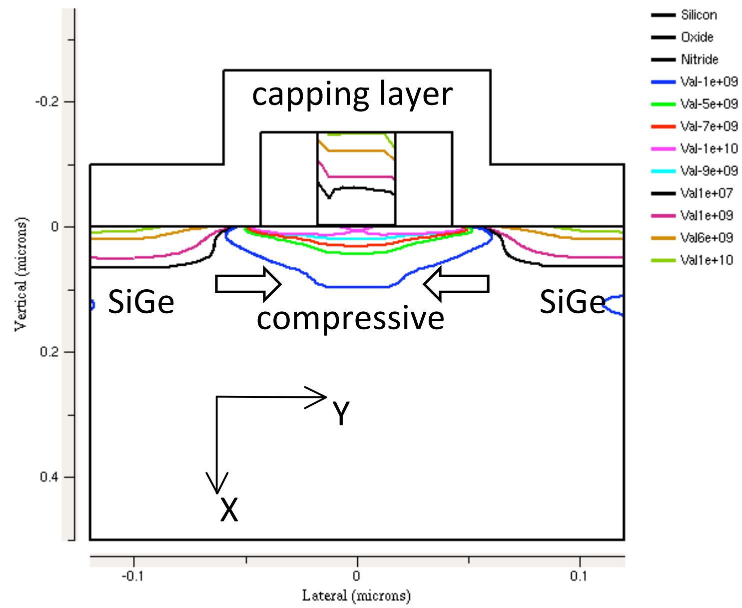
- To enhance channel mobility, PMOS strain processing includes embedded SiGe in the source/drain regions and compressive capping layers.
- FLOOXS predicts strain/stress profiles where the channel stress is ~1 GPa



Cheng, *et al.* IEDM 2007



Horstmann, *et al.* IEDM 2005

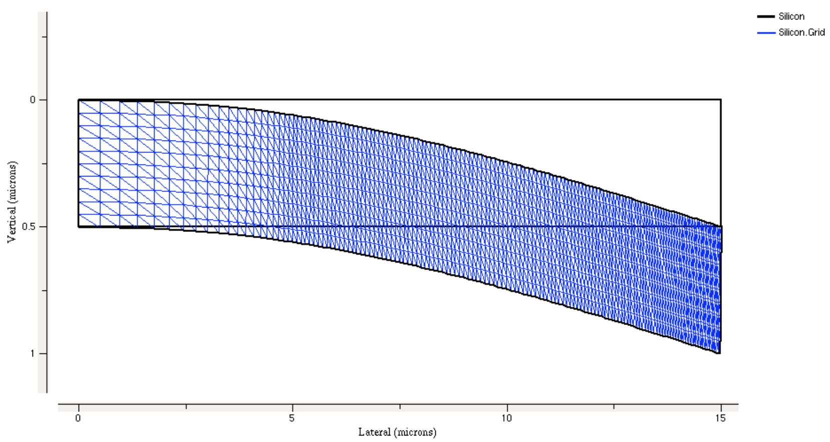


FLOOXS predicted stress profile [dyne/cm2]
(YY component - channel direction)

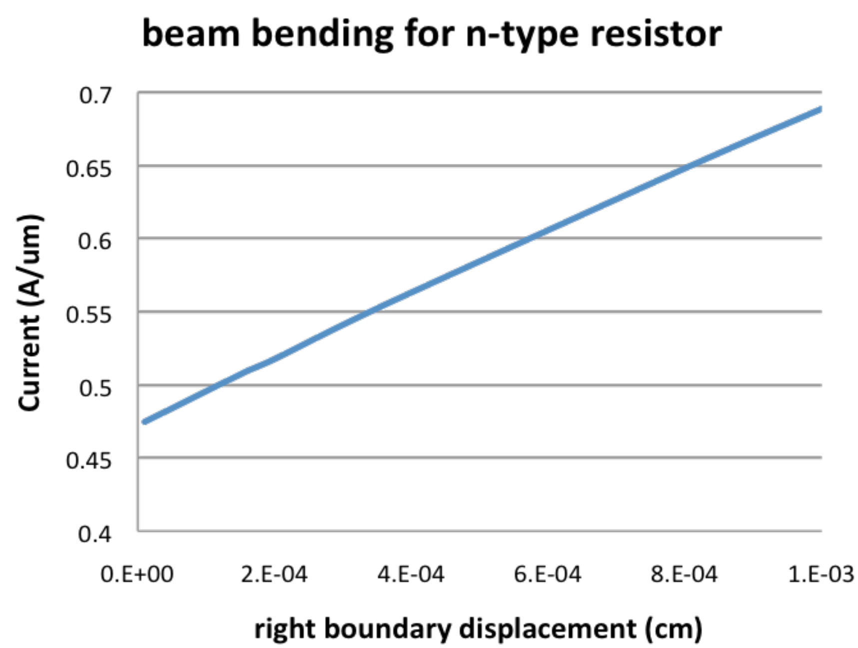
Piezoresistance example

- Silicon beam with an n-type surface
- Bending induces tensile stress at the surface resulting in a increase in mobility and current.

$$J_X(\sigma) \cong \left(1 + \frac{-\Delta\mu_{xx}}{\mu_{xx}}\right) J_X(0) = \left(1 + \pi_{11}\sigma_{xx}\right) J_X(0)$$

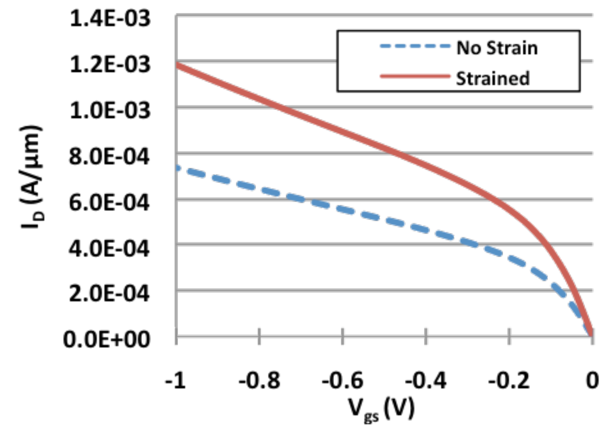


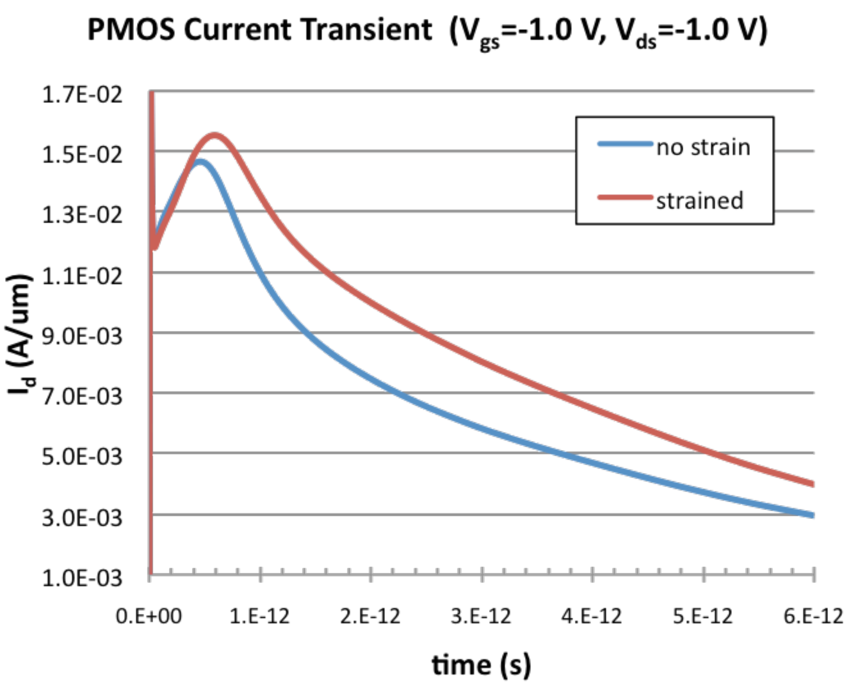
FLOOXS beam bending example

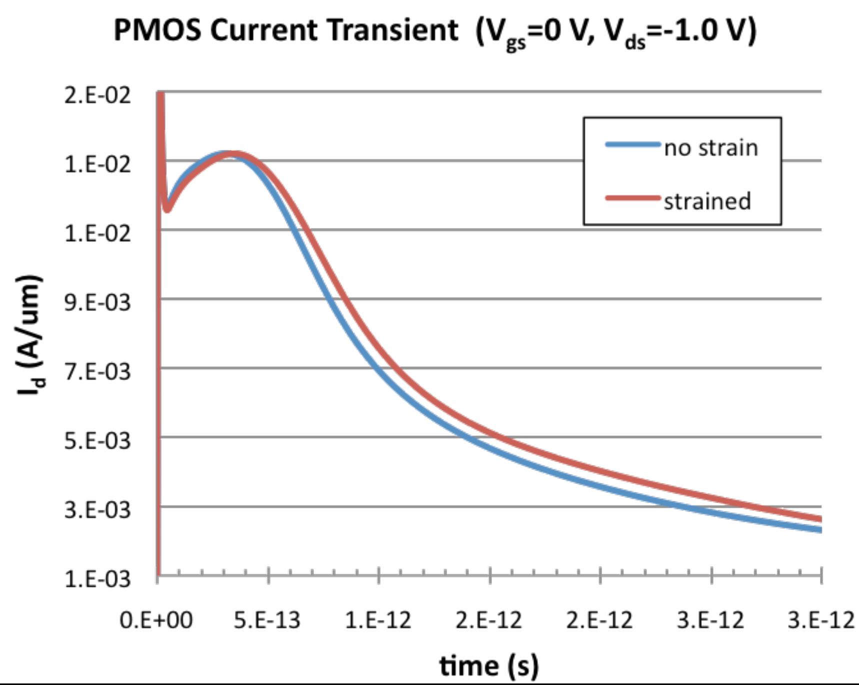


Strained PMOS Simulations

- PMOS with L_{gate}=30 nm
- <110> channel orientation
- 2007 ITRS dimensions
- Charge strike dist. in drain

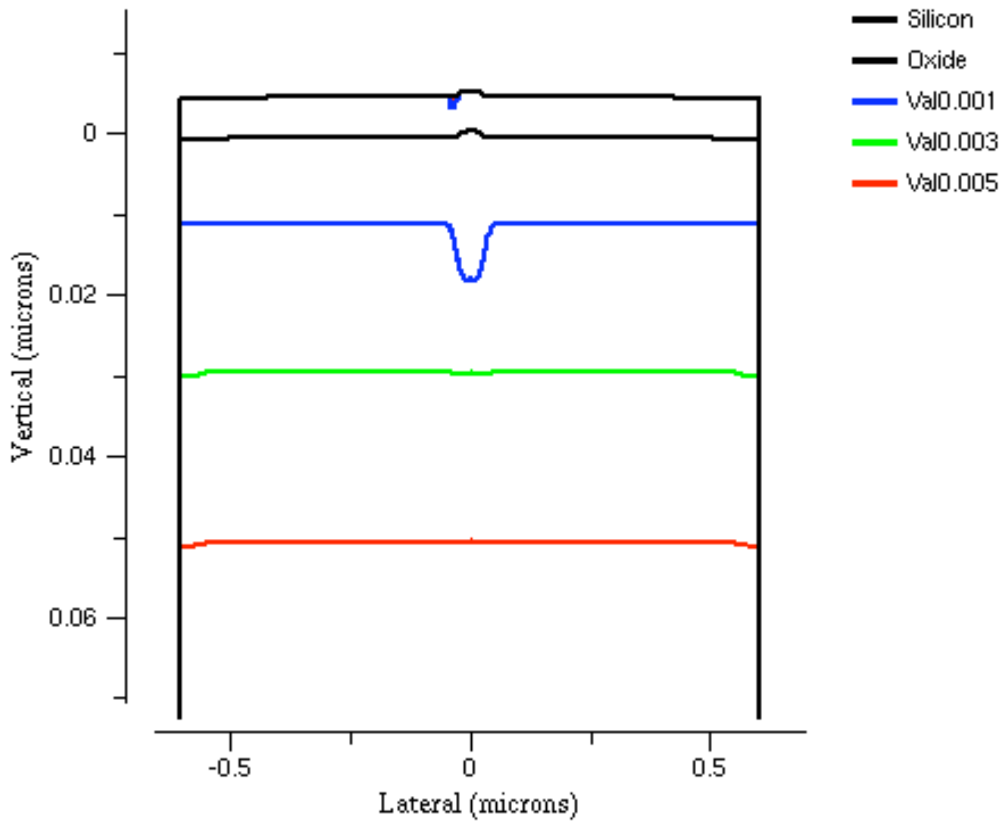






Inverse Piezoelectric Effect Calculation

- Mechanical Simulation with Piezo Terms
- Simple test case - MOS Cap on Piezo Material
- Asymmetry in the strain due to change in direction in the horizontal field across the gate



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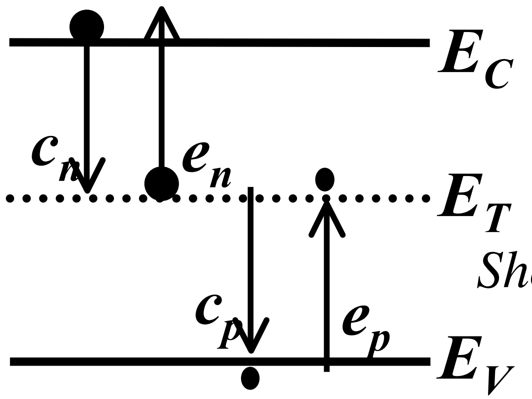
Noise Simulation Progress to date

The current version of FLOODS was upgraded, with the help of Juan Sanchez PhD, to include

- Small signal AC simulation for calculating channel and transfer impedance and transconductance
- Velocity fluctuation and defect noise simulation
- External circuit elements

Modeling of defects



- Random carrier transitions between continuum states (E_C, E_V) and localized defect states.

Shockley-Read-Hall Model

Four basic equations with one trap level added, 3+N with N trap levels:

$$F_\psi = -\frac{d^2\psi}{dr^2} - \frac{q}{\varepsilon}\left[p - n + N_D^+ - N_A^- - n_t\right] = 0$$

$$F_n = \frac{dn}{dt} - \frac{1}{q}\nabla \cdot \boldsymbol{J}_n - g_n + r_n - \gamma_n(\boldsymbol{r},t) = 0$$

$$F_p = \frac{dp}{dt} + \frac{1}{q}\nabla \cdot \boldsymbol{J}_p - g_p + r_p + \gamma_p(\boldsymbol{r},t) = 0$$

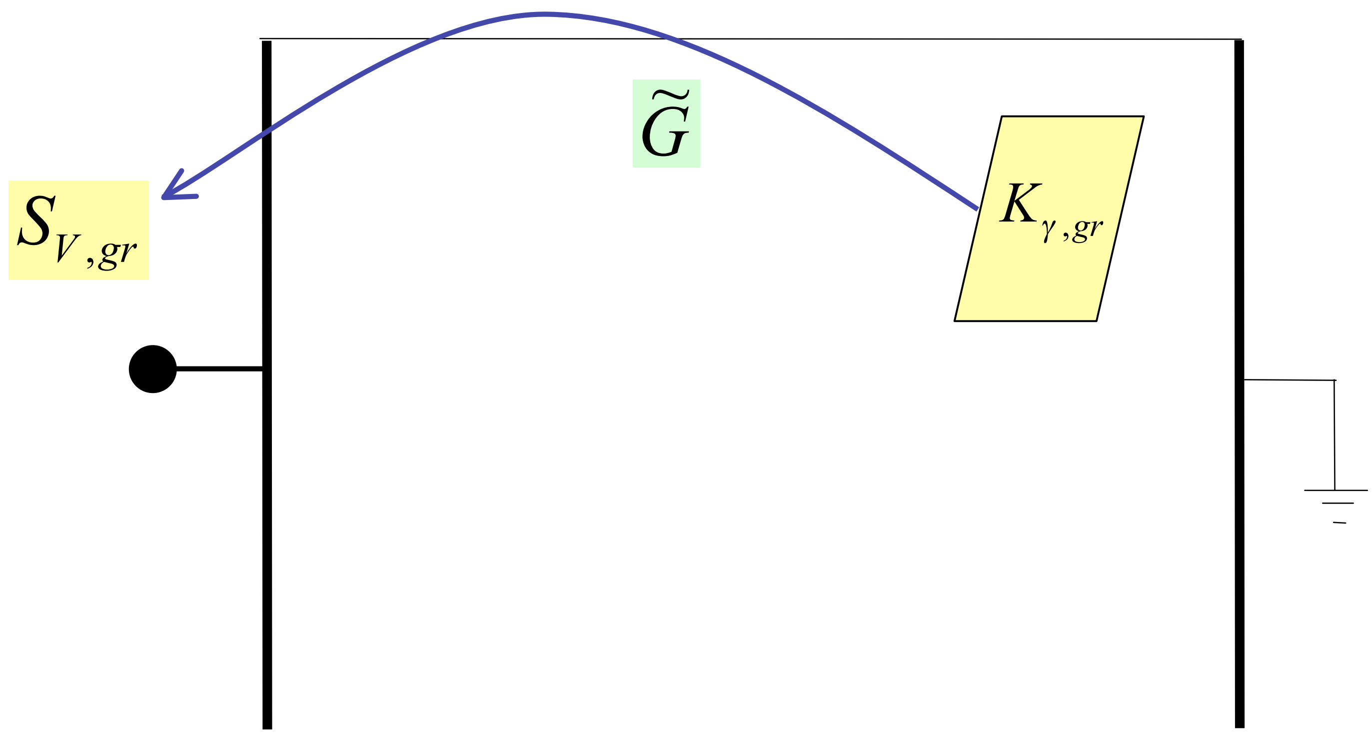
$$F_{n_t} = \frac{dn_t}{dt} + g_n - r_n - g_p + r_p - \gamma_t(\boldsymbol{r},t) = 0$$

Noise terms

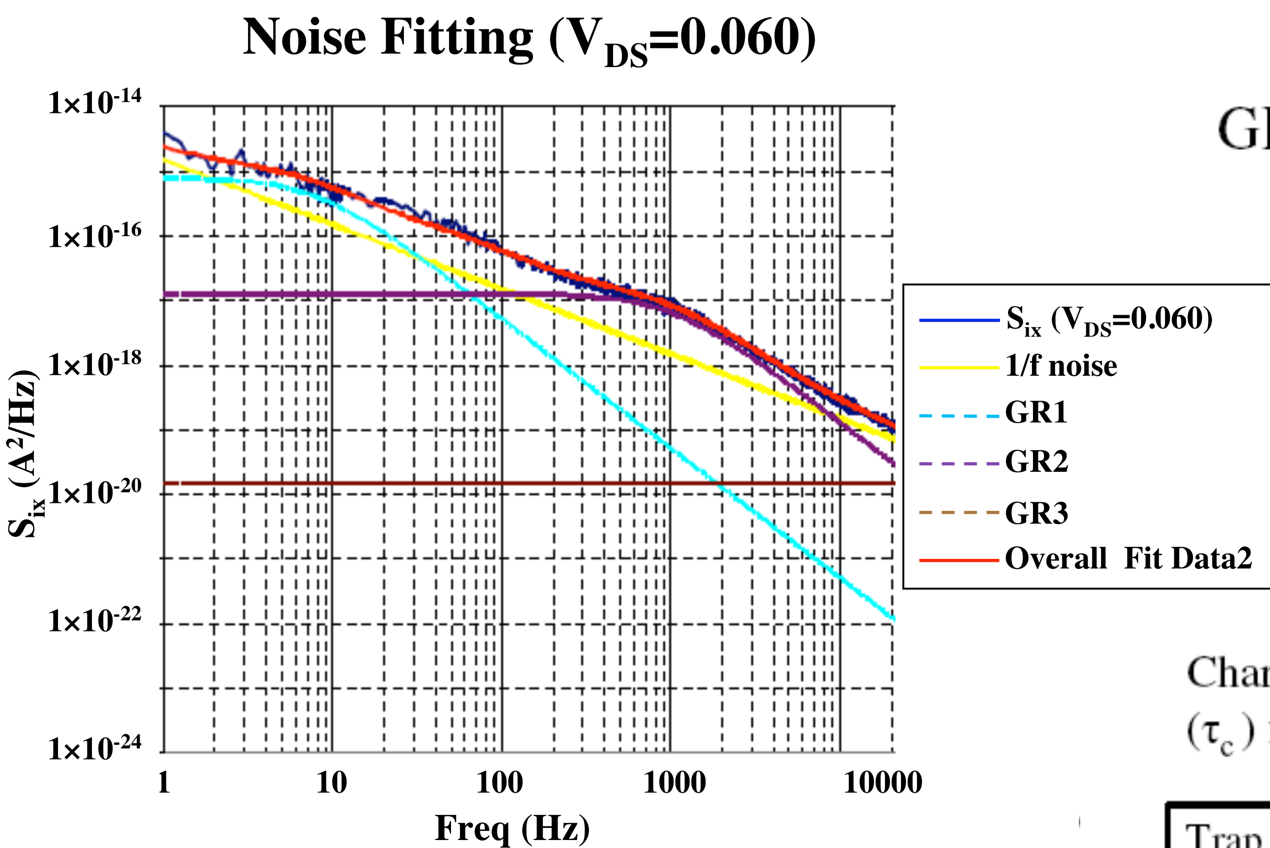
- Fluctuations in n_t perturbs the charge in the system
  - Add noise terms to trapped electron continuity equation
- Fluctuations in n and p
  - Add noise terms to both the electron and hole continuity equations
- Noise source terms are expressed in defect activation energy, defect density and capture cross-section.
- G-R noise source strength in each differential volume is mapped to the external contact using scalar Green's function (in contrast with Diffusion and Hooge noises which use vector Green's function)

$$S_{V,gr} = \sum_{i=1}^{Ntrap} \sum_{\alpha=\psi,n,p} \widetilde{G}_{\alpha} K_{\gamma_{\alpha i},\gamma_{\alpha i}} \widetilde{G}^{*}_{\beta} dr$$

Noise Source Mapping



Noise Decomposition Normal S-D Operation



GR Noise and 1/f Noise

$$S_{ID}(f) = \frac{q\mu\alpha_H I_D V_{DS}}{L^2 f}$$

Approximate Hooge Parameter $\boxed{\alpha_H = 2.56\times10^{-3}}$

Characteristic Relaxation Time (τ_c) for GR Noise

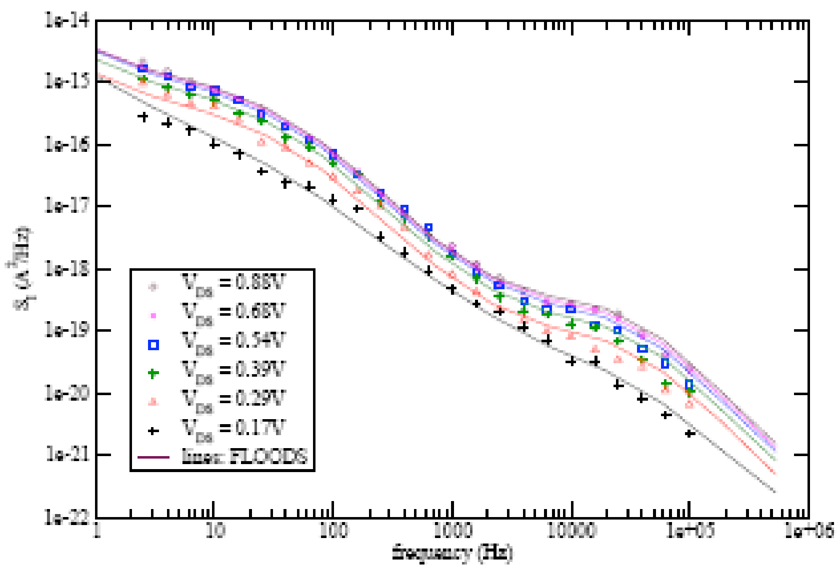
Trap 1	Trap 2	Trap 3
14.4 ms	132.7 µs	1.06 µs

Simulation of defect noise

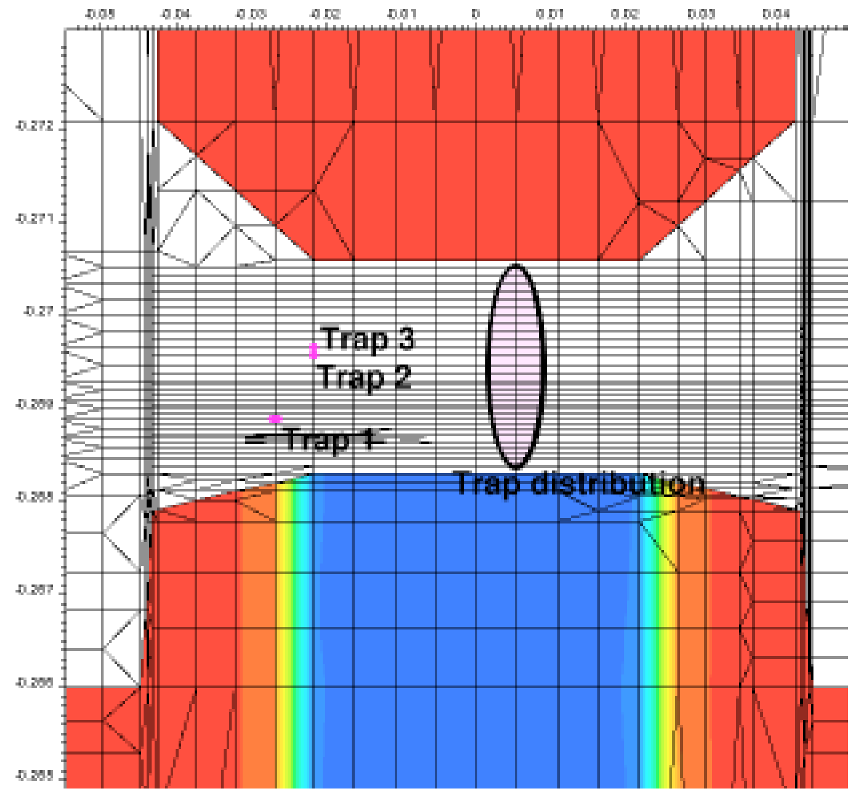
Brute Force Approach: Start with a 4x4 Jacobian matrix system with 1 trap level, or a (3+N) x (3+N) system with N trap levels. The noise Jacobian matrix becomes

$$\begin{bmatrix} \frac{dF_\psi}{d\psi} & \frac{dF_\psi}{dn} & \frac{dF_\psi}{dp} & \frac{dF_\psi}{dn_t} \\ \frac{dF_n}{d\psi} & \frac{dF_n}{dn} + j\omega & \frac{dF_n}{dp} & \frac{dF_n}{dn_t} \\ \frac{dF_p}{d\psi} & \frac{dF_p}{dn} & \frac{dF_p}{dp} + j\omega & \frac{dF_p}{dn_t} \\ \frac{dF_{n_t}}{d\psi} & \frac{dF_{n_t}}{dn} & \frac{dF_{n_t}}{dp} & \frac{dF_{n_t}}{dn_t} + j\omega \end{bmatrix} \begin{bmatrix} \tilde{\psi} \\ \tilde{n} \\ \tilde{p} \\ \tilde{n}_t \end{bmatrix} = \begin{bmatrix} 0 \\ \tilde{\gamma}_n \\ -\tilde{\gamma}_p \\ \tilde{\gamma}_{n_t} \end{bmatrix}$$

Example: 3.2µm x 90nm bulk nMOSFET



Low frequency measured and simulated noise data



Graphical depiction of ***Noise Producing*** oxide trap locations on mesh for simulating the low frequency noise features. Location 1 has 4 traps, locations 2 and 3 0.5 traps each.

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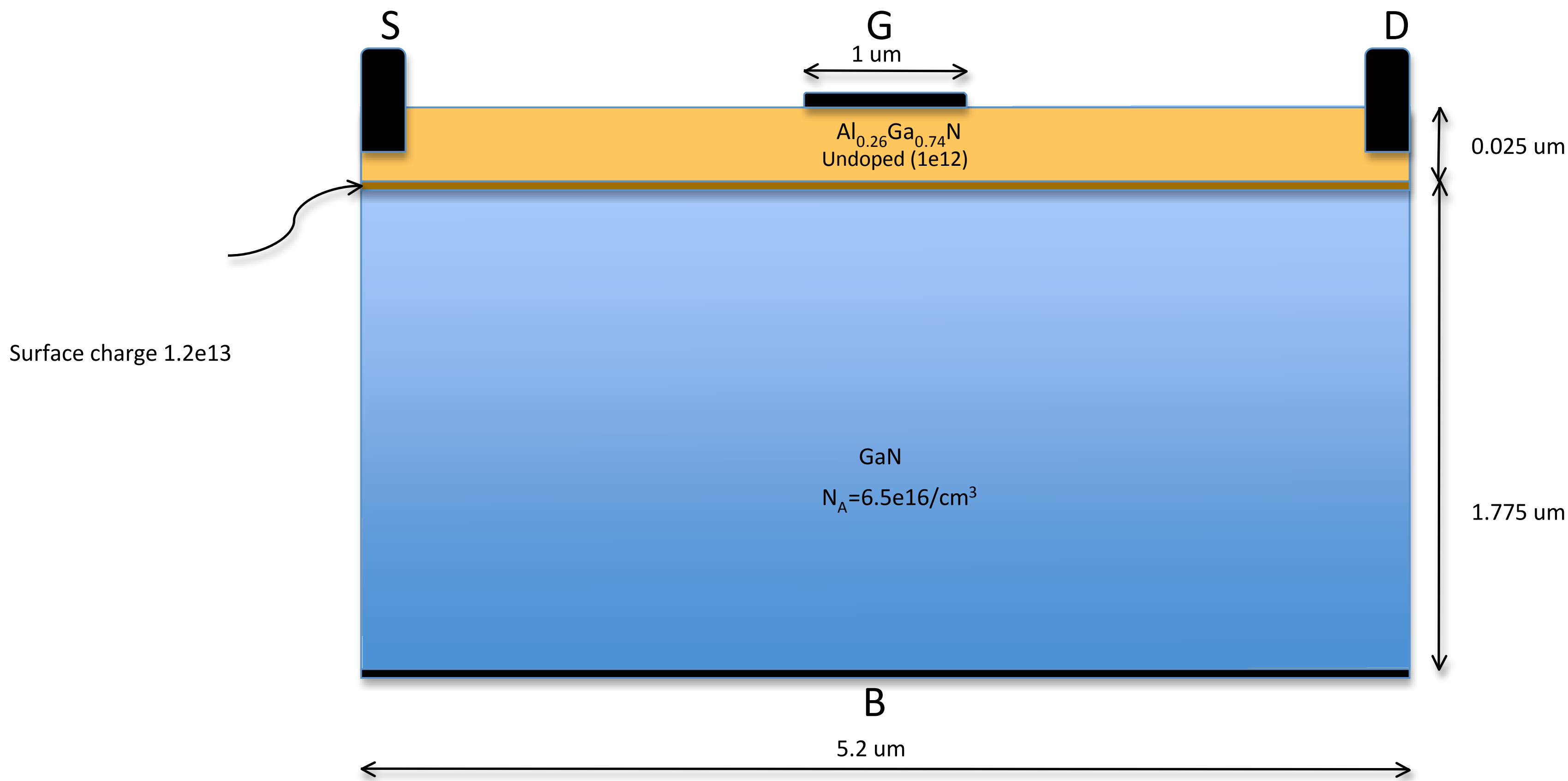
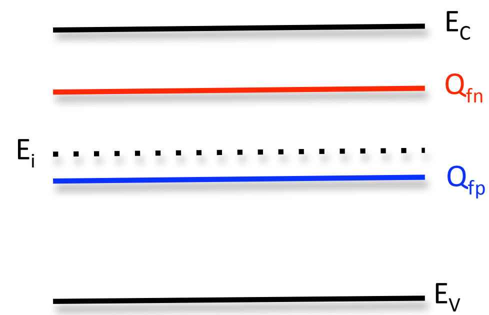
HEMT Structure



[Not to scale]

Quasi-Fermi Approach

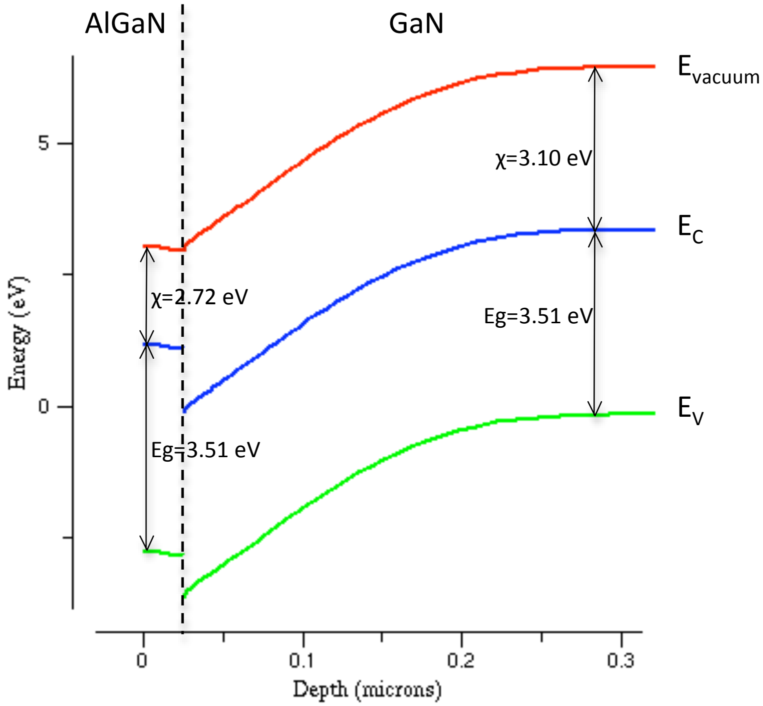
- Quasi-Fermi levels are energy levels used to specify the carrier concentrations under *non*equilibrium conditions
  - Similar to Fermi level for equilibrium conditions
  - Two energy levels
    - Qfn: Quasi-Fermi level for electrons
    - Qfp: Quasi-Fermi level for holes
- Streamlined approach for heterostructure device simulation
  - Helps define electron and hole concentrations continuously across the interface
  - Quasi-Fermi level that varies with position indicates current flow
- Affects:



Carrier Concentration Equations $p=N_V e^{(Ev-Qfp)/kT}$ $n=N_c e^{(Qfn-Ec)/kT}$

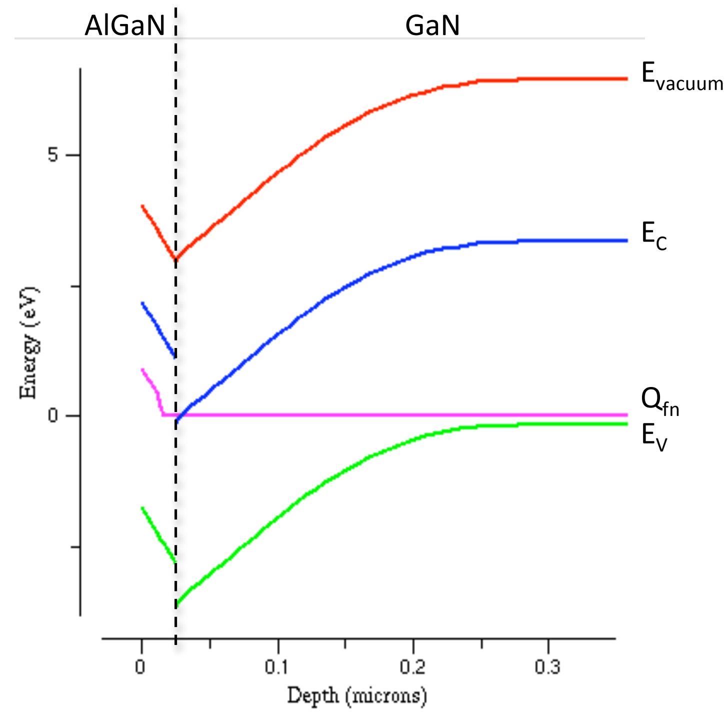
Carrier Continuity Equations $\frac{dp}{dt}=\mu_p p \nabla Q_{fp}$ $\frac{dn}{dt}=\mu_n n \nabla Q_{fn}$

Energy Band Diagram



At equilibrium

V_G=0V V_D=0V



After gate bias

V_G=-1V V_D=0V

Reverse bias at Schottky G contact

Bands bend up to achieve pinch-off

Mobility Model

Future work on strain-induced polarization demands a robust mobility model which includes field dependence

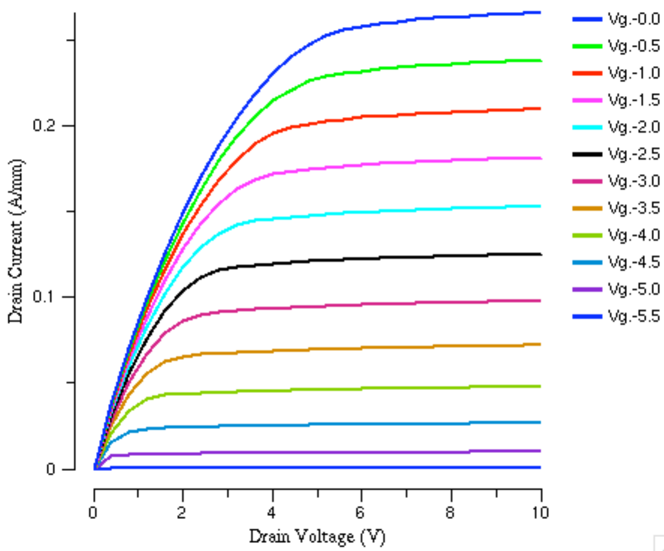
- Farahmand, et. al., IEEE Trans. Elec. Dev., 48, no. 3, 2001
- Low-field mobility
  - Drift-diffusion
    - Influence of temp (T) and ionized impurity concentration (N)
    - μ_{max}, μ_{min}, α, β_{1-4}
      - Parameters from Farahmand

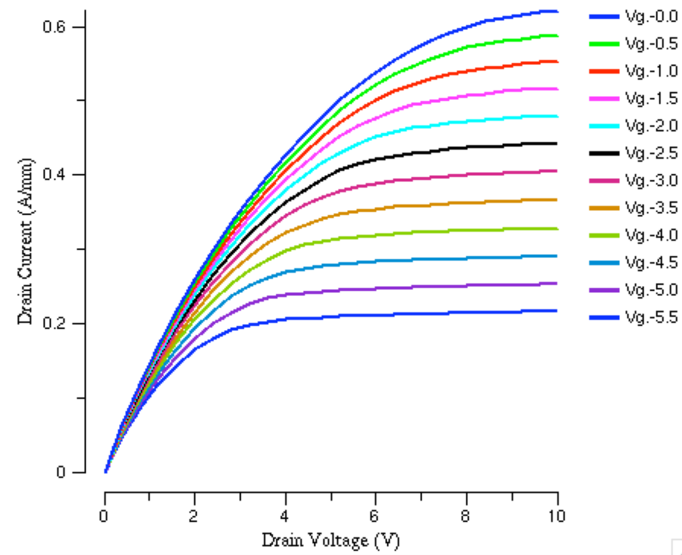
$$\mu_0(T, N) = \mu_{min}\left(\frac{T}{300}\right)^{\beta_1} + \frac{(\mu_{max} - \mu_{min})\left(\frac{T}{300}\right)^{\beta_2}}{1 + \left[\dfrac{N}{N_{ref}\left(\frac{T}{300}\right)^{\beta_3}}\right]^{\alpha(T/300)^{\beta_4}}}$$

- High-field mobility
  - Low-field + field dependent mobility
    - E: Electric field
    - E_c, v_{sat}, a, n_1, n_2
      - Parameters from Farahmand

$$\mu = \frac{\mu_0(T, N) + v^{sat}\dfrac{E^{n1-1}}{E_c^{n_1}}}{1 + a\left(\dfrac{E}{E_c}\right)^{n_2} + \left(\dfrac{E}{E_c}\right)^{n_1}}$$

Interface Charge Effect





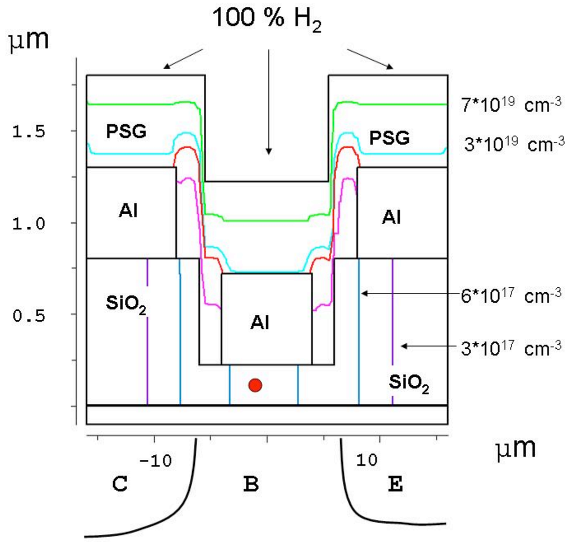
Interface charge 1.2e13 | Interface charge 2.0e13

- Interface charge added with easy single command line
- Positive charge at interface draws in electrons
- Increased interface charge leads to larger 2DEG current and higher v_{Dsat}
- Link to strain calculations

Hydrogen Trapping Simulation

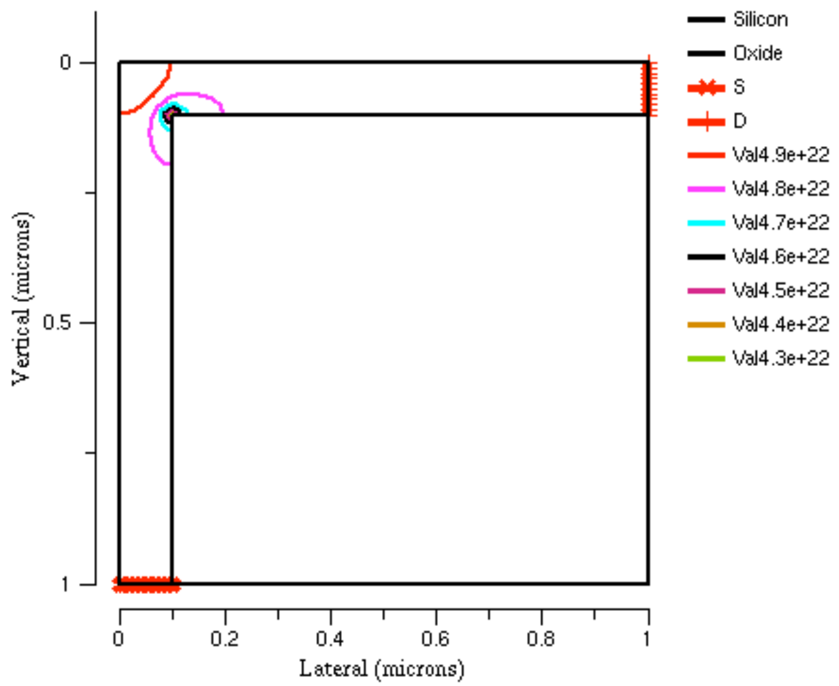
TNS, TBP
Vanderbilt + UF

- Simulate Device in Quasi-Steady State
  - Electrons and Holes equilibrate quickly
  - Similar to assumption in process simulation
- Generation Events Triggered by
  - Mechanical Stress
  - Current Flow / Electric Field
- Simultaneous solutions
  - Point Defects / Defect Cluster / Interface Capture
  - Hydrogen



Material Flow Simulation

- Crude electromigration simulation
- Density is lowest where field is highest (corner)
- Field driven kickout mechanism



Conclusions

- Modeling Integrated
  - Fundamental Physics k•p feeds TCAD
- Experimentally Integrated
  - Failure Mechanism Identification feeds M&S
  - Electrical Measurement feeds

- Connect strain calculations
- Temperature / Traps